

Geometric Quantum Gates, Composite Pulses, and Trotter-Suzuki Formulas

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(Dated: September 14, 2010)

We show that all geometric quantum gates (GQG's in short), which are quantum gates only with geometric phases, are robust against control field strength errors. As examples of this observation, we show (1) how robust composite rf-pulses in NMR are geometrically constructed and (2) a composite rf-pulse based on Trotter-Suzuki Formulas is a GQG.

PACS numbers: 03.65.Vf, 82.56.-b, 82.56.Jn, 03.67.-a, 03.65.-w

Geometric phases have been attracting a lot of attention from the view point of the foundation of quantum mechanics and mathematical physics [1, 2, 3, 4]. Recently, a geometric quantum gate (GQG in short), which is a quantum gate only with geometric phases, is spotlighted in quantum information processing [5, 6], because they are expected to be robust against noise. Although its robustness has not yet been generally confirmed [7, 8, 9, 10, 11, 12], some GQG's are robust against certain types of fluctuations [13].

On the other hand, composite rf-pulses are extensively employed in NMR [14, 15], which are robust against systematic errors of the system. Note that rf-pulses are means for controlling spin states and have direct correspondence to quantum gates. Most of composite rf-pulses in NMR are designed with the knowledge of initial states, and thus it is often not replaceable with simple pulses. However, there are *fully compensating* composite rf-pulses that are replaceable with simple pulses without further modifications of other pulses, and thus are compatible in use for quantum computation, as demonstrated in ion traps [16] and Josephson junctions [17] as well as in NMR [18].

In this letter, we discuss the relation between fully compensating composite quantum gates which is robust against control field strength errors and non-adiabatic GQG's with Aharonov-Anandan (AA) phases [19]. Let us define an ideal single-qubit operation

$$R(\mathbf{m}, \theta) = \exp(-i\theta \frac{\mathbf{m} \cdot \boldsymbol{\sigma}}{2}), \quad (1)$$

where we take the natural unit system in which $\hbar = 1$. \mathbf{m} is a unit vector ($\in \mathbb{R}^3$), while $\boldsymbol{\sigma}$ is a standard Pauli matrix vector such that $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. θ represents a control field strength. Note that θ and \mathbf{m} are both constant. A real erroneous operation $\tilde{R}(\mathbf{m}, \theta)$ with a systematic control field strength error is modeled as follows.

$$\tilde{R}(\mathbf{m}, \theta) = R(\mathbf{m}, \theta(1 + \epsilon)) = R(\mathbf{m}, \theta) + O(\epsilon),$$

where $\epsilon \ll 1$ is an unknown fixed parameter that represents the error. If we find a series of operations $\tilde{R}(\mathbf{m}_j, \theta_j)$

(\mathbf{m}_j and θ_j are constant), such that

$$\prod_{j=1}^N \tilde{R}(\mathbf{m}_j, \theta_j) = R(\mathbf{m}, \theta) + O(\epsilon^2), \quad (2)$$

we call it a fully compensating composite quantum gate which is robust against a control field strength error.

In order to proceed our discussion, we first review an AA phase that appears under non-adiabatic cyclic time evolution of a quantum system [19] and a GQG with it for a single qubit [13]. The qubit state $|\mathbf{n}(t)\rangle (\in \mathbb{C}^2)$ at $t (\in [0, T])$ corresponds to the Bloch vector $\mathbf{n}(t) = \langle \mathbf{n}(t) | \boldsymbol{\sigma} | \mathbf{n}(t) \rangle (\in \mathbb{R}^3)$. Suppose that the Hamiltonian $H(t)$ generates a cyclic time evolution such that $|\mathbf{n}(T)\rangle = e^{i\gamma} |\mathbf{n}(0)\rangle$ ($\gamma \in \mathbb{R}$). The AA phase γ_g is defined as [19]

$$\gamma_g = \gamma - \gamma_d, \quad (3)$$

where

$$\gamma_d = - \int_0^T \langle \mathbf{n}(t) | H(t) | \mathbf{n}(t) \rangle dt \quad (4)$$

is a dynamic phase. Next, suppose $|\mathbf{n}_+(0)\rangle$ and $|\mathbf{n}_-(0)\rangle$ are two states satisfying (a) $\langle \mathbf{n}_+(0) | \mathbf{n}_-(0) \rangle = 0$ (or, $\mathbf{n}_+(0) = -\mathbf{n}_-(0)$) and (b) $|\mathbf{n}_\pm(T)\rangle = e^{i\gamma_\pm} |\mathbf{n}_\pm(0)\rangle$, where $\gamma_\pm \in \mathbb{R}$. An arbitrary quantum state $|\mathbf{n}(0)\rangle$ is expressed as $|\mathbf{n}(0)\rangle = a_+ |\mathbf{n}_+(0)\rangle + a_- |\mathbf{n}_-(0)\rangle$, where $a_\pm = \langle \mathbf{n}_\pm(0) | \mathbf{n}(0) \rangle$. We call $\mathbf{n}_\pm(0)$ as a basis Bloch vector associated with $H(t)$. The initial state $|\mathbf{n}(0)\rangle$ is transformed into the final state

$$|\mathbf{n}(T)\rangle = a_+ e^{i\gamma_+} |\mathbf{n}_+(0)\rangle + a_- e^{i\gamma_-} |\mathbf{n}_-(0)\rangle.$$

Thus, the time evolution operator U at $t = T$ generated by $H(t)$ ($t \in [0, T]$) is rewritten as

$$U = e^{i\gamma_+} |\mathbf{n}_+(0)\rangle \langle \mathbf{n}_+(0)| + e^{i\gamma_-} |\mathbf{n}_-(0)\rangle \langle \mathbf{n}_-(0)|. \quad (5)$$

Eq. (5) is regarded as a quantum gate with an AA geometric phase, when the dynamic component of γ_\pm is vanishing.

Let us discuss the following Hamiltonian

$$H(\mathbf{m}, \theta) = \theta \frac{\mathbf{m} \cdot \boldsymbol{\sigma}}{2} \frac{1}{T}, \quad (6)$$

at $t \in [0, T]$ [20]. Applying this Hamiltonian for $[0, T]$, $R(\mathbf{m}, \theta)$ (Eq. (1)) is obtained. The dynamic phase γ_d generated by $H(\mathbf{m}, \theta)$ at $t \in [0, T]$ for the system starting from $|\mathbf{n}\rangle$ is given as [13]

$$\begin{aligned}\gamma_d &= -\int_0^T \langle \mathbf{n} | H(\mathbf{m}, \theta) | \mathbf{n} \rangle dt \\ &= \langle \mathbf{n} | H(\mathbf{m}, \theta) T | \mathbf{n} \rangle = -\frac{\theta}{2} \mathbf{m} \cdot \mathbf{n}.\end{aligned}\quad (7)$$

The state $|\pm \mathbf{m}\rangle$ is a cyclic state for $H(\mathbf{m}, \theta)$ and there is no other cyclic state except for $|\pm \mathbf{m}\rangle$ for $H(\mathbf{m}, \theta)$ if $\theta \pmod{2\pi} \neq 0$. By using $|\pm \mathbf{m}\rangle$, $R(\mathbf{m}, \theta)$ is rewritten as

$$R(\mathbf{m}, \theta) = e^{-i\theta/2} |\mathbf{m}\rangle \langle \mathbf{m}| + e^{i\theta/2} |-\mathbf{m}\rangle \langle -\mathbf{m}|,$$

like Eq. (5). We may call $R(\mathbf{m}, \theta)$ as a dynamic phase gate by contrasting a GQG.

We are ready to discuss a composite quantum gate $\prod_{j=1}^N \tilde{R}_j$, such that $\prod_{j=1}^N R_j = R(\mathbf{n}_0, \theta)$. $\tilde{R}(\mathbf{m}_j, \theta_j)$ and $R(\mathbf{m}_j, \theta_j)$ are abbreviated to \tilde{R}_j and R_j , respectively. We assume that each duration of R_j is T_j and thus the associated Hamiltonian for R_j is $H_j = \theta_j \frac{\mathbf{m}_j \cdot \boldsymbol{\sigma}}{2} \frac{1}{T_j}$. By ignoring $O(\epsilon^2)$,

$$\begin{aligned}&\prod_{j=1}^N \tilde{R}(\mathbf{m}_j, \theta_j) \\ &= \prod_{j=1}^N R(\mathbf{m}_j, \theta_j (1 + \epsilon)) \\ &= R(\mathbf{n}_0, \theta) + \sum_{j=1}^N R_N \dots R_j (R(\mathbf{m}_j, \theta_j \epsilon) - I) \dots R_1 \\ &= R(\mathbf{n}_0, \theta) + \sum_{j=1}^N R_N \dots R_j \left(I - i\epsilon \theta_j \frac{\mathbf{m}_j \cdot \boldsymbol{\sigma}}{2} - I \right) \dots R_1 \\ &= R(\mathbf{n}_0, \theta) - i\epsilon \sum_{j=1}^N R_N \dots R_j (H_j T_j) \dots R_1,\end{aligned}$$

where I is the identity operator for a qubit. We calculate the expectation value of the second term for $|\mathbf{n}_0\rangle$ that is a cyclic state for both $R(\mathbf{n}_0, \theta)$ and $\prod_{j=1}^N R_j$ by definition.

$$\begin{aligned}&\langle \mathbf{n}_0 | - \sum_{j=1}^N R_N \dots R_j H_j T_j R_{j-1} \dots R_1 | \mathbf{n}_0 \rangle \\ &= -e^{-i\theta/2} \sum_{j=1}^N \langle \mathbf{n}_{j-1} | H_j T_j | \mathbf{n}_{j-1} \rangle\end{aligned}\quad (8)$$

where $|\mathbf{n}_j\rangle = \prod_{k=1}^j R_k |\mathbf{n}_0\rangle$. Note that $\langle \mathbf{n}_0 | R_N \dots R_j = e^{-i\theta/2} \langle \mathbf{n}_{j-1} |$ by definition of $\prod_{j=1}^N R_j$.

If $\prod_{j=1}^N \tilde{R}_j$ is a fully compensating composite quantum gate which is robust against a control field strength error, $\sum_{i=1}^N R_N \dots R_j (H_j T_j) \dots R_1$ should vanish by definition,

or by Eq. (2). And thus, Eq. (8) should vanish. On the other hand, $-\langle \mathbf{n}_{j-1} | H_j T_j | \mathbf{n}_{j-1} \rangle$ is a dynamic phase $\gamma_{d,j}$ accumulated during the j 'th operation R_j . Then, we conclude that

$$\sum_{j=1}^N \gamma_{d,j} = 0,$$

for the cyclic state $|\mathbf{n}_0\rangle$. It is also obvious that $\prod_{j=1}^N R_j$ generates no dynamic phase when starting from $|\mathbf{n}_0\rangle$ where $\langle -\mathbf{n}_0 | \mathbf{n}_0 \rangle = 0$. Therefore,

$$\prod_{j=1}^N R_j = e^{i\gamma_g} |\mathbf{n}_0\rangle \langle \mathbf{n}_0| + e^{-i\gamma_g} |-\mathbf{n}_0\rangle \langle -\mathbf{n}_0|,$$

where $\gamma_g = -\theta/2$ is a geometric phase. In other words, *a fully compensating composite quantum gate without a dynamic phase is always robust against a control field strength error.*

We, however, note that not-all robust composite quantum gates are regarded as GQG's with AA-phases. For example, CORPSE pulses [21] are not regarded as GQG's since we can only define cyclic states that acquire dynamic phases after operations. These composite rf-pulses rely on the non-linearity of pulse responses.

We now discuss some concrete examples of composite quantum gates in terms of vanishing dynamic phases.

No dynamic phases during a composite quantum gate: We discussed $R(\mathbf{x}, \pi/2)R(\mathbf{y}, \pi)R(\mathbf{x}, \pi/2)$, where $\mathbf{x}(\mathbf{y})$ is the unit vector along the x (y) axis [13]. This composite rf-pulse is very special in the sense that no dynamic phases are generated for its cyclic states at any moment of operation R_j . We noticed the importance of dynamic phases in quantum operations [13] and now extend this observation so that the sum of dynamic phases is important.

SCROFULOUS pulse and W1 correction sequence: Cummins, Llewellyn, and Jones showed the systematic method how to construct a composite rf-pulses called SCROFULOUS pulses

$$R(\mathbf{m}_1, \theta_1)R(\mathbf{m}_2, \pi)R(\mathbf{m}_1, \theta_1) = R(\mathbf{x}, \theta), \quad (9)$$

where $\mathbf{m}_i = (\cos \phi_i, \sin \phi_i, 0)$ and θ_1 is an rotation angle of the first and third pulses [21]. We take \mathbf{x} for simplicity, but generalization from \mathbf{x} to \mathbf{m} in the xy-plane should be trivial. We discuss another way to construct them in terms of dynamic phases. From Eq. (9) [22],

$$\langle \mathbf{x} | R(\mathbf{m}_1, \theta_1)R(\mathbf{m}_2, \pi)R(\mathbf{m}_1, \theta_1) | \mathbf{x} \rangle = e^{-i\theta/2}.$$

Then, we obtain

$$\cos \theta_1 = \frac{\tan(\phi_1 - \phi_2)}{\tan \phi_1}, \quad (10)$$

$$\sin \frac{\theta}{2} = \frac{\sin(\phi_1 - \phi_2)}{\sin \phi_1}. \quad (11)$$

From the condition that the sum of dynamic phases is zero [23] and Eq. (10), we obtain

$$2\theta_1 \cos(\phi_1 - \phi_2) + \pi = 0. \quad (12)$$

By solving Eqs. (10-12)[24], we obtain the same results as in Ref. [21].

A W1 sequence [21] which corrects $R(\mathbf{x}, \theta)$ is

$$U_{W1} = R(\mathbf{m}_1, \pi)R(\mathbf{m}_2, 2\pi)R(\mathbf{m}_1, \pi) = I.$$

Here, we take $\phi_1 = \pm \arccos(-\theta/(4\pi))$ and $\phi_2 = 3\phi_1$. U_{W1} is rewritten as

$$U_{W1} = e^{i\gamma_{W1}}|\mathbf{x}\rangle\langle\mathbf{x}| + e^{-i\gamma_{W1}}|-\mathbf{x}\rangle\langle-\mathbf{x}|,$$

where $\gamma_{W1} = \gamma_{g,W1} + \gamma_{d,W1} = 0$ and $\gamma_{g,W1}(\gamma_{d,W1})$ is a geometric (dynamic) phase. Since $\gamma_{d,W1} = -\gamma_{g,W1} = \theta/2$, the composite quantum gate $R(\mathbf{x}, \theta/2)U_{W1}R(\mathbf{x}, \theta/2)$ becomes a GQG.

Composite rf-pulse based on Trotter-Suzuki formula: Brown, Harrow, and Chuang discussed a systematic method, named Trotter-Suzuki method, to construct a composite rf-pulses [25]. We re-examine this method in terms of a dynamic phase. Let us consider a composite quantum gate that is equivalent to $R(\mathbf{x}, \theta)$. Erroneous rotation $\tilde{R}(\mathbf{x}, \theta) = R(\mathbf{x}, \theta)R(\mathbf{x}, \theta\epsilon)$ is able to be compensated when $R(\mathbf{x}, \theta\epsilon)$ is approximately canceled by another erroneous rotations $\tilde{R}(\mathbf{m}', \theta')$'s. According to Trotter-Suzuki Formulas [26], we can select A_i 's so that

$$\begin{aligned} R(\mathbf{x}, -\theta\epsilon) &= \exp\left(-i\left(-\theta\frac{\sigma_x}{2}\right)\epsilon\right) \\ &= \prod_{i=1}^N \exp(-iA_i\epsilon) + O(\epsilon^2) \end{aligned}$$

where $-\theta(\sigma_x/2) = \sum_{i=1}^N A_i$ ($N \geq 2$). Now, we take $N = 2$ (the smallest number) for simplicity and call A_i as A_{\pm} . We require that $|\mathbf{x}\rangle$ is the cyclic state for $\exp(-iA_{\pm})$ as well as $R(\mathbf{x}, \theta)$. A_{\pm} that satisfies these conditions is, for example,

$$A_{\pm} = -2\pi \frac{\mathbf{m}_{\pm} \cdot \boldsymbol{\sigma}}{2},$$

where $\mathbf{m}_{\pm} = \cos\phi \mathbf{x} \pm \sin\phi \mathbf{y}$ and $\phi = \cos^{-1}(\theta/4\pi)$. Since

$$\begin{aligned} R(\mathbf{m}_+, -2\pi(1+\epsilon))R(\mathbf{m}_-, -2\pi(1+\epsilon)) \\ = \exp(-iA_+\epsilon)\exp(-iA_-\epsilon), \end{aligned}$$

a robust composite quantum gate

$$R(\mathbf{m}_+, -2\pi)R(\mathbf{m}_-, -2\pi)R(\mathbf{x}, \theta)$$

is constructed. Let us examine the condition $-\theta(\sigma_x/2) = A_+ + A_-$ for using the Trotter-Suzuki formula. By taking into account that $|\mathbf{x}\rangle$ is the cyclic state for both $R(\mathbf{x}, \theta)$ and $R(\mathbf{m}_{\pm}, -2\pi)$,

$$\begin{aligned} 0 &= \langle\mathbf{x}|\theta\frac{\sigma_x}{2} + A_+ + A_-|\mathbf{x}\rangle \\ &= \langle\mathbf{x}|\theta\frac{\sigma_x}{2}|\mathbf{x}\rangle + \langle\mathbf{x}|R(\mathbf{x}, -\theta)A_-R(\mathbf{x}, \theta)|\mathbf{x}\rangle \\ &\quad + \langle\mathbf{x}|R(\mathbf{x}, -\theta)R(\mathbf{m}_-, 2\pi)A_+R(\mathbf{m}_-, -2\pi)R(\mathbf{x}, \theta)|\mathbf{x}\rangle. \end{aligned}$$

In other words, the condition for using the Trotter-Suzuki formula ($-\theta(\sigma_x/2) = A_+ + A_-$) is equivalent that the sum of dynamic phases during the composite quantum gate is vanishing.

We show that all GQG's with Aharonov-Anandan phases are fully compensating composite quantum gates that are robust against control field strength errors. We also show (1) how SCROFULOUS pulses and W1 sequences [21] are geometrically constructed and (2) the condition for using the Trotter-Suzuki formulas [25, 26] is equivalent that the sum of dynamic phases in a composite quantum gate is vanishing. Although the discussed case is not general, our observation provides a physical view on the Trotter-Suzuki formulas. In conclusion, *(no)dynamic phases are important to obtain reliable quantum gates.*

We would like to thank Mikio Nakahara, Yukihiro Ota, and Tsubasa Ichikawa for discussions. This work was supported by ‘‘Open Research Center’’ Project for Private Universities: Matching fund subsidy from Ministry of Education, Culture, Sports, Science and Technology.

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- $$\cos \frac{\theta}{2} = -\cos(\phi_1 - \phi_2) \sin \theta_1,$$
- $$\sin \frac{\theta}{2} = \cos \theta_1 \cos \phi_1 \cos(\phi_1 - \phi_2) + \sin \phi_1 \sin(\phi_1 - \phi_2).$$
- [23] The condition on the dynamic phases is
- $$2\theta_1 \cos \phi_1 + \pi \cos \phi_1 \cos(\phi_1 - \phi_2) + \pi \cos \theta_1 \sin \phi_1 \sin(\phi_1 - \phi_2) = 0$$
- by employing Eq. (7). From Eq. (10) and this condition, we get Eq. (12).
- [24] We start from $\cos^2(\phi_1 - \phi_2) + \sin^2(\phi_1 - \phi_2) = 1$ and substitute Eqs. (10-12) into it. Then, we obtain
- $$\frac{1}{\theta_1} \sin \theta_1 = \frac{2}{\pi} \cos(\theta/2),$$
- and
- $$\phi_1 = \arccos \left(\frac{-\pi \cos \theta_1}{2\theta_1 \sin(\theta/2)} \right),$$
- $$\phi_2 = \phi_1 - \arccos \left(\frac{-\pi}{2\theta_1} \right).$$
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